A Computational Workbench Environment For Virtual Power Plant Simulation

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ABSTRACT

In this paper we describe our progress toward creating a computational workbench for performing virtual simulations of Vision 21 power plants. The workbench provides a framework for incorporating a full complement of models, ranging from simple heat/mass balance reactor models that run in minutes to detailed models that can require several hours to execute. This paper provides an overview of a process workbench for a conventional PC power plant developed during the past year and our current efforts at developing a workbench for a gasifier based energyplex configuration.

INTRODUCTION

Virtual simulation of advanced systems will play an important role in reducing the time, cost and technical risk of developing a DOE Vision 21 energyplex [DOE, 1999]. It is our belief that virtual simulations of these systems will require the use of a broad range of component models that will require new ways of conducting these simulations to perform them in a cost effective manner.

In our DOE Vision 21 project, Reaction Engineering International (REI) is developing a computational workbench that will provide a ***framework*** for integrating the range of models and visualization methods that will be required to perform simulations to predict energyplex performance and emissions. The workbench is being developed as a tightly integrated problem solving environment, with plug and play functionality, that contains an array of tools and models that communicate in a seamless manner. The workbench is designed for use by the non-specialist and provides the capability to interrogate a simulation at multiple levels of detail. The models contained in the workbench can range in complexity from simple heat/mass balance models to sophisticated CFD based models. Through the course of this program, models will be created for simulating key energy plant components, including boilers, gasifiers, fluidized beds, combustors, fuel cells and clean-up process components. Some of these models will tax the limits of the computer power readily available to most engineers.

The workbench is being constructed using the SCIRun software system. SCIRun is a continuously evolving product of the Scientific and Computational Imaging group, headed by Prof. Chris Johnson, in the Department of Computer Science at the University of Utah (UU/SCI). From inception, SCIRun has been designed in an object-oriented manner with the intent of supporting interdisciplinary projects in which High Performance Computing (HPC) models are needed. SCIRun places no inherent limitations on the physics, numerical technique or programming language used within a model. SCIRun supports component-based software techniques and allows for distributed computing. In addition, it is possible to interface additional software packages to SCIRun. To enhance the inherent visualization capabilities of SCIRun, REI has incorporated the OpenDX data visualization software package into the workbench. OpenDX is a popular package being used by researchers in a variety of disciplines that must visualize, analyze and explore large data sets.

For Year One, the focus of our project has been to develop a prototype workbench based on a conventional pulverized coal combustion plant, the DOE Low Emissions Boiler System Proof of Concept (LEBS-POC) facility. LEBS-POC is a system with which we are familiar and thus provides an opportunity to quickly evaluate many software design issues for the workbench. The prototype workbench uses a CFD model for the radiant furnace box. Reactor models have been implemented to simulate steam generation, the air pre-heater, NOx reduction with a Selective Catalytic Reduction (SCR) unit and particulate removal using a baghouse or an Electric Static Precipitator (ESP). In Year Two and Year Three, the focus of the project will be on creating models for gasifier-based systems and implementing these models into an improved workbench.

In this paper we describe our work effort for Year One and outline our plans for future work. Discussed, in order, are: our workbench concept; the software systems and software design used within the workbench; the functionality of the workbench; the models contained within the Year One prototype workbench; a demonstration of using the workbench to evaluate the impact on downstream operations of changes in the boiler firing conditions; and last, the planned model development to occur in Year Two and Year Three that will lead to simulating a Vision 21 energyplex system.

COMPUTATIONAL WORKBENCH – OVERVIEW

A *workbench environment* is more than just a set of software tools with a graphical user interface (GUI). The workbench contains all of the tools required for problem setup, running the models (steady or transient) and analyzing the simulation results. The computational models included in the workbench can be of arbitrary complexity and can be implemented in a wide variety of programming languages.

Traditionally, power plant simulation has been performed using either spreadsheet, flowsheet or CFD models. Spreadsheet models typically utilize algebraic models, or correlations, based on historical data (or multiple runs of more detailed models) to create a simple representation of the plant components. Spreadsheet-based models are easy to use, run quickly but contain only limited accuracy with respect to predicted performance. The IECM tool [http://www.IECM-online.com] would be an example of a spreadsheet model. A flowsheet system model typically contains mass and energy balance models, also called process or reactor models, for the equipment components within the plant. Although reactor models are limited in the physics that are considered, they are more accurate than correlations and run quickly. Flowsheets are good tools for analyzing the impact of equipment or process changes, evaluating control strategies and studying the dynamic response of the plant to upset conditions. Example commercial packages for flowsheet systems are Aspen, Hysys and GTPro. All of the commercial packages have simple interfaces and extensive user support. Computational Fluid Dynamic (CFD) models are a third type of model. CFD based models provide much more detailed information about the component because they include the impact of localized mixing and heat transfer within the reactor. However, at present CFD models are typically used only for key plant components due to the computational expense and difficulty in using these more sophisticated models. In addition, the CFD models are typically run in a “stand-alone” mode and the impact of upstream or downstream equipment must be accounted with additional computations performed by the user, off-line from the CFD simulation.

The computational workbench being developed in our Vision 21 project provides a significant step forward from analysis, or plant simulation, tools currently available. In final form, our process workbench will include component models ranging from simple reactor models to detailed, CFD-based models. Where feasible, multiple choices for model types will be provided. The reactor models will include simple algebraic models as well as mass/energy balance models. Where appropriate, reaction kinetics will also be included. The use of reactor models created as look-up tables from CFD modeling results will also be investigated. For key components in the plant, CFD models will be included. For all of the models, simple User Input panels will be provided that contain appropriate default values. The workbench will contain the flexibility for the engineer to choose whether to utilize a reactor or CFD model for any particular component. The CFD models will be implemented in such a manner to make these models to be easy to use. Using a combination of different model types will result in a cost effective analysis of a plant configuration.

WORKBENCH – SOFTWARE: SCIRun and OpenDX

The latest SCIRun software represents the state-of-the-art in computational problem solving environments and is particularly well suited for cutting-edge, interdisciplinary computational projects [http://www.sci.utah.edu]. Basic features and functionality of SCIRun and how these are being utilized to create our process workbench have been previously described elsewhere [Bockelie, 2001a], [Bockelie, 2001b] and thus are not presented here. Below we describe our efforts during the last year at incorporating OpenDX into SCIRun and in exploring software protocols to use when integrating models into the workbench.

OpenDX for Visualization

Creating a link between SCIRun and OpenDX gives the workbench user access to the large range of visualization and data analysis capabilities possible with OpenDX. DX was originally developed by IBM. Its long history as a commercial software package shows in its polished core visualization capabilities and extensive documentation. Since being released to open source, DX has been widely accepted as the visualization package of choice for research groups in national laboratories, universities and large industrial research laboratories. The large user base for DX ensures that modules exist to manipulate, transform, process, realize, render and animate data based on points, lines, areas, volumes, images or geometric primitives. These modules can be quickly arranged to provide popular data analysis tools, such as: display point values (point probe); one (XY), two (carpet/surface plots) and three dimensional plots; line and solid shaded contours, iso-surface extraction, data and vector value slices, solid particle trajectories through flow fields. More complicated networks can be built for nearly every conceivable visualization task. Thus, OpenDX provides all of the capabilities of commercially available data visualization packages, plus additional state-of-the-art capabilities to visualize, interrogate, explore and analyze data sets. Further information about OpenDX is available on the web at: http://www.opendx.org. The coupling between the workbench and OpenDX is accomplished using a library called DXLink. This package is distributed with the OpenDX software suite. DXLink allows a remote application to maintain fine-grained control of all aspects of OpenDX. Anything that can be accomplished using the dedicated DX user-interface can also be accomplished remotely with DXLink. An important design consideration of the SCIRun-to-DX link is the visualization user interface. Forcing the user to move between the SCIRun user interface panels and those of DX would be cumbersome and confusing. To eliminate this difficulty, the user interface for the OpenDX visualization engine has been written using TCL/TK and integrated with the SCIRun workbench. This provides the user a seamless user interface experience, while DXLink is being used to transparently move information and commands to and from DX. The visualization module is accessed by selecting a button labeled "3D" located on a module icon. The visualization user interface has a "look and feel" comparable to that employed in commercial CFD visualization tools. Non-specialist users are not being aware that OpenDX is being used. However, sophisticated workbench users have access to powerful data visualization and analysis tools.

Model Integration

Proper model integration techniques can provide significant advantages, most notably model interoperability among the various Vision 21 teams and third-party developers. In the following, we detail the techniques used for model integration for the Year One prototype workbench (Workbench I), along with plans for a more sophisticated approach for the Vision 21 Energyplex workbench (Workbench II). A robust and functional model integration paradigm is a key element of Workbench II being developed during Year Two and Year Three of this program.

Workbench I Model Integration Paradigm: During the development of the LEBS Workbench I, we have focused on a proven, traditional method of integrating the models into the SCIRun environment. This has involved the creation of C++ wrapper classes, which encapsulate the model of interest. This wrapper performs several functions, including abstracting model inputs and outputs, providing execution controls and providing SCIRun-to-model communication mechanisms. The instantiation of the resulting wrapper class yields a SCIRun compliant module, which is capable of being composed as part of a dataflow network program. While using the aforementioned mechanism of model integration was the natural choice for the LEBS Workbench I, it does have shortcomings as a final solution. The most significant issue is that of interoperability of the wrapped models. This method generates modules which will only function within the SCIRun system. It is not possible to move these modules to other frameworks or to use modules developed for other frameworks inside SCIRun. In addition, the method places limits on model programming languages and provides no inherent parallelism.

Workbench II Model Integration Paradigm: To address the functional requirements of Workbench II, model integration will need to be performed using the methods of component architectures with standardized interfaces. Component architectures alone offer numerous advantages when compared with conventional programming techniques. These advantages include programming language and platform independence, location transparency (and hence parallelism) and reuse. When these core advantages of component architectures are coupled with standardized interfaces, reuse becomes interoperability.

For Workbench II, our intention is to allow interoperability of models through two emerging component architecture-based standards: **CAPE-OPEN** and **CCA**. CAPE-OPEN [http://www.colan.org] is a set of standards created to facilitate the use of COM and CORBA component software for process engineering problems. The CAPE-OPEN standard is specifically designed for process engineering problems and provides numerous capabilities. This standard has been well received by the process engineering community. Numerous simulation environments have already been modified for CAPE compliance (Aspen Plus, HYSYS). Although CAPE provides much functionality and interoperability, it alone does not fully address the needs of Workbench II model integration. CAPE has limitations due to its narrow targeting of process engineering problems, and its reliance on COM and CORBA which are currently not acceptable for high performance computing applications. To address the need for component architecture for HPC, the Common Component Architecture (CCA) Forum was created [http://www.acl.lanl.gov/cca-forum/]. The creation of this forum was inspired by the DOE2000 initiative. The specification created by this group provides the benefits of the standard business oriented component architectures (interoperability, language independence, parallel capabilities), while addressing the issues of high-performance computing such as parallel communication channels between components and other elements required for dealing with extremely large data sets. By supporting both the CAPE-OPEN and CCA standards, Workbench II would benefit from the development of models in both the HPC and process engineering arenas. Plans to make SCIRun CCA 0.5 compliant and to implement CAPE functionality are being formulated.

WORKBENCH – USER INTERFACE AND FUNCTIONALITY

Illustrated in Figure 1 is a SCIRun interface for the LEBS Proof of Concept (POC) unit (described below). Each rectangle in this figure denotes a module (or plant component) with encapsulated functionality. The pipes that connect the modules (or boxes) denote the transfer of model data between modules. Data flows from one component to the next, much in same way that “material” flows through an engineering process flow diagram. Conversion modules are used to allow “data massaging” as the data flows from one component to the next. These are needed because not all models require the same level of detail for their input data (i.e., a module using a detailed CFD simulation is connected to a module using a simple heat/mass balance model). SCIRun provides the flexibility to perform all of the required functions. The inputs for any component model can be inherited from an upstream device or entered directly via input dialog boxes that can contain pull down menus, type-in boxes, radio buttons and menu selections as per standard GUI operation. The visual programming capability within SCIRun allows an engineer to modify the *dataflow network* of the virtual power plant in a user-friendly manner. Additional modules can be instantiated at any time during a computational analysis, as can the connections between modules. The interface to SCIRun can best be described as a graphical programming environment with true plug-and-play functionality.

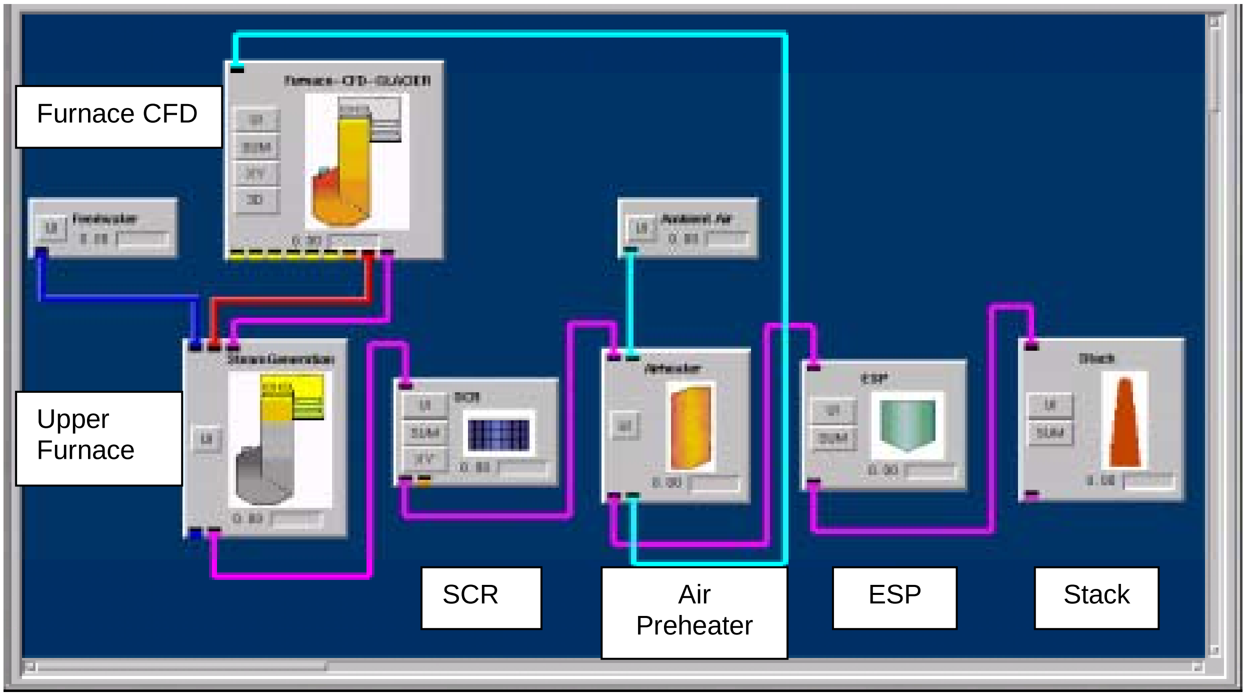

Figure 1. User Interface for prototype workbench (Workbench I).

Provided below are brief descriptions of the techniques provided for the user to input model data, view model outputs and interrogate intermediate data.

Model Inputs: Located on each SCIRun module is a button labeled “UI”. Selecting the UI button will cause a TK-based user input dialog box to appear on the screen. Using this dialog, the engineer can alter the model parameters that would impact module performance. The input dialog uses a combination of simple type-in boxes and other standard user-interface elements that request information in terms (and units) typically used in the combustion community. To make operation of the workbench as robust and user-friendly as possible, default values are provided for all model inputs, and all inputs are checked for errors prior to allowing the user to close the dialog.

Model Outputs: By selecting the appropriate buttons on the module icons, model results can be viewed in different ways. The most basic form of output is a simple summary table of values (SUM button). Typically the summary data consists of the 5-10 key items for that model. For a CFD furnace model, typical items displayed in the summary data window would be average values at the furnace exit for the gas temperature, gas composition (O_2, CO, NO), fuel conversion (%), etc. Model output information can also be displayed as XY, or 1D, plots (XY button). Results for modules containing a CFD model can be displayed using 3D visualization methods (3D button). The OpenDX package provides the user the ability to perform all of the standard CFD visualization methods (see Figure 2b). The combination of OpenDX and SCIRun also provides the ability to perform some low cost virtual reality methods, such as stereoscopic visualization using “stereo glasses”, volume rendering and “fly-through” scenarios. The ability of SCIRun to “bridge” to other software packages also opens the possibility of interfacing the workbench to other virtual reality tools. Some possible linkages are: 3DstudioMax, a professional 3D modeling package that can be used to create plant walk-through scenarios; and VR-Juggler, a software package used to drive large scale immersive environments such as the C-2, C-4 and C-6 at the Iowa State University Virtual Reality Applications Center.

Port Interrogation: Port Interrogation provides the user with a mechanism, or tool, to display all of the data contained within the gas and solids stream data structure that is passed between different workbench modules through the data pipes. With this tool, the user can view detailed information about the composition, temperature, etc. for the gas and solids at any point within the module network. The Port Interrogation can be performed for any module by placing the cursor over the desired data port and performing a right mouse click.

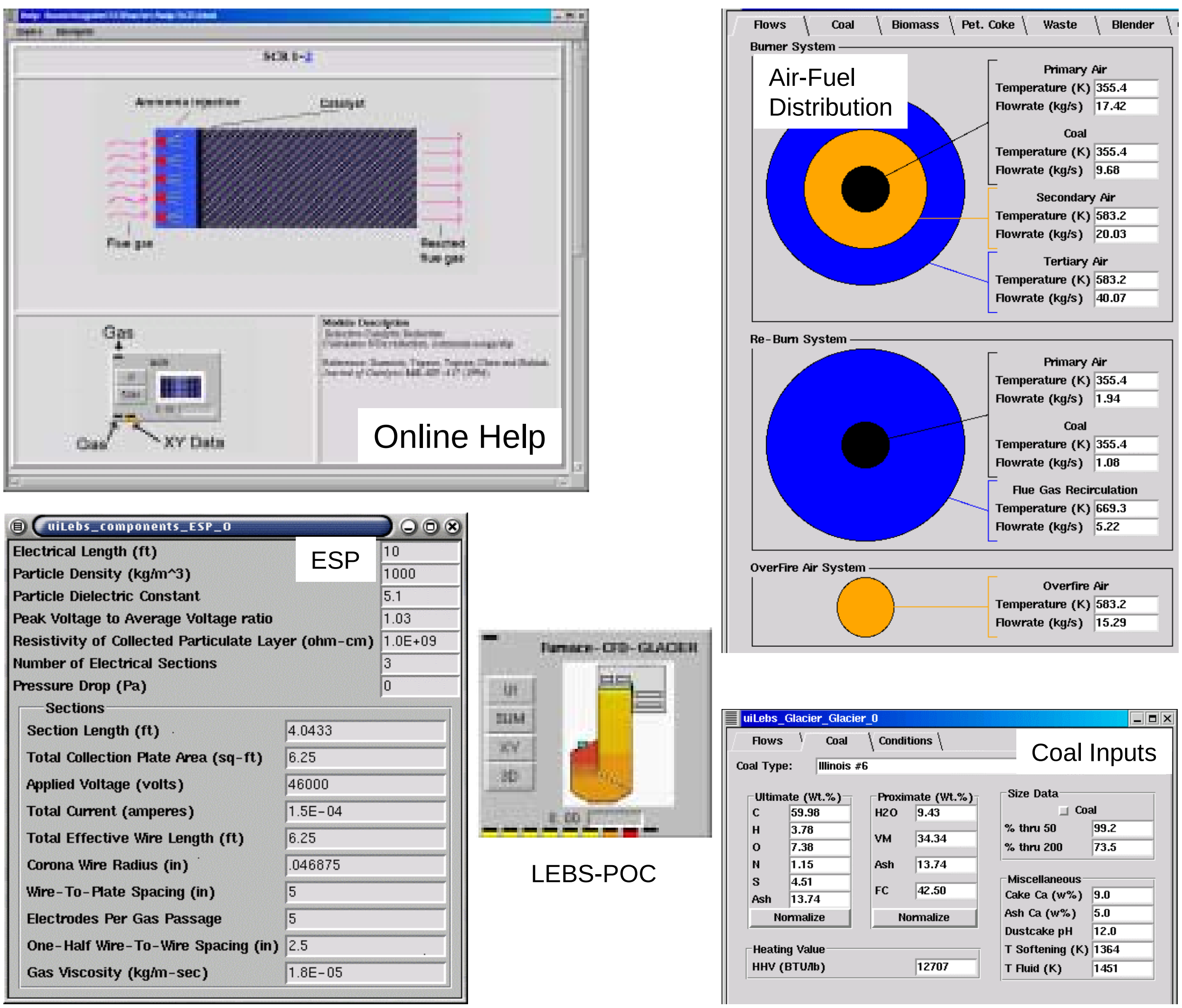

Figure 2. Windows showing online help, input dialog boxes for different modules.

Online Help System: A key element of a successful workbench is an easily accessible online help system. Such a system allows a user to quickly answer questions regarding model inputs, outputs, usage and capabilities. To address this need, we have implemented a help system that uses HyperHelp, an iTCL html viewer, to display hypertext help files for each module. The Help content includes: instructions on usage of the module; a description of the module ports; a picture of the module user interface; and a description of the fields in the UI. To access help for a given module, the user simply uses the mouse to right-click on the module, and selects the "Help" item from the pop-up menu. Because the module documentation is created using HTML, the online help system is easy to create and maintain using the plethora of tools available for web development. Figure 2 shows examples for online help and input dialog windows for some modules.

WORKBENCH ENVIRONMENTS

In Year One of our program we developed a prototype workbench for a current generation PC plant. The selected plant configuration is based on the DOE Low Emissions Boiler System Proof of Concept (LEBS-POC) facility. With the start of Year Two of our program, our effort is now focused on developing a workbench for a gasifier-based energyplex. A key aspect of the Year Two effort will be to develop a user-configurable, CFD-based gasifier model. Below we describe our efforts on each of the workbench systems.

Prototype Workbench

The LEBS-POC is a nominally 90 MW, down-fired unit. It contains four low NOx burners in a staggered arrangement in a U-shaped, wet bottom boiler and has provisions for OFA and reburning. The LEBS-POC plant configuration, as represented in the workbench, is shown in Figure 1. The prototype workbench uses a CFD model for the radiant furnace box. Reactor models have been implemented to simulate steam generation, the air pre-heater, NOx reduction with a Selective Catalytic Reduction (SCR) unit and particulate removal. Modules for a baghouse and an Electro-Static Precipitator (ESP) have been provided for modeling particulate removal.

For the firebox, two CFD modules have been implemented. One module is based on *GLACIER*, a comprehensive two phase CFD-based combustion code. *GLACIER* has been used by REI to model a variety of utility boiler configurations [http://www.reaction-eng.com]. At present, *GLACIER* is limited to performing steady-state simulations. A module has also been implemented for *AIOLOS*, a comprehensive CFD combustion code developed at the University of Stuttgart, that can be used for performing steady or unsteady simulations of coal fired utility boilers.

GLACIER POC Furnace Module (Steady-State): The *GLACIER* CFD code is a comprehensive CFD modeling code that can be used to model a broad range of turbulent reacting flows. It is capable of modeling two-phase fuels for either gas-particle or gas-liquid applications. For establishing the basic combustion flow field, full equilibrium chemistry is employed. To compute NOx and other trace species, finite rate chemistry effects can be included in a post-processor mode. Turbulence chemistry coupling is accomplished using PDF methods. An important aspect of GLACIER is the tight coupling used between the dominant physics for utility boiler applications: turbulent fluid mechanics, radiation heat transfer, chemical reactions and particle/droplet dynamics. Further information on GLACIER is available at http://www.reaction-eng.com/combustion.htm.

AIOLOS POC Furnace Module (Transient/Steady-State): The *AIOLOS* CFD code is a comprehensive CFD modeling code that can be used to model a broad range of turbulent reacting flows. It can be used to model two-phase fuel applications, using either Eulerian-Eulerian or Eulerian-Lagrangian methods. *AIOLOS* employs an EDC technique for turbulence chemistry coupling. It can employ multi-domain grids and perform time dependent coal combustion simulations using either implicit or explicit time stepping. It can be used on virtually any level of hardware or operating systems. *AIOLOS* is parallel-capable on both SMP and distributed architectures. It can be executed on single or dual CPU PCs/workstations and PC clusters, and has been tuned for use on supercomputers. Further information on AIOLOS can be found on the web at: http://www.ivd.uni-stuttgart.de/english/aiolos_e_fh.html.

Upper Furnace Module**:** A simple model has been implemented to compute the steamside and CO burnout in the upper, or convective pass, of the furnace. For the steamside model, the steam flow rate and exit steam conditions are computed from thermodynamic steam calculations coupled with an integrated heat transfer rate to the steam from the CFD model for the POC boiler. The model is based on a tube bank heat exchanger model, with correlations taken from [B&W, 1992]. Included in the model is a stream property code. The module was tested by comparing predicted values versus design data for the LEBS-POC.

SCR Module**:** A plug flow SCR model has been developed based on the microkinetic mechanism of Dumesic et al. (1996) (also known as the Topsoe mechanism) for NOx reduction with vanadia/titania catalysts. This is the most common SCR catalyst used by utilities and is the catalyst that will be used in the LEBS-POC facility. The model was verified through comparisons of predicted values and values presented in Dumesic et al. (1993).

Air Heater Module: The air preheater is a heat exchanger that uses hot effluent gas from the furnace to heat the secondary and tertiary combustion air and over fire air (OFA). The air heater module was created by re-using the tube bank heat transfer model developed for the steam side module.

Baghouse Module: The baghouse model is based on a simple zero dimensional reactor model that computes capture efficiency and pressure drop, based on the amount of trapped solids. The pressure drop calculations are important to establish fan requirements. The baghouse model used here is based on a model provided to REI by the Southern Research Institute [Pontius, Robinson & Vann Bush, 1992].

ESP Module: The ESP model implemented into the workbench is based on a model provided by Clean Air Engineering (CAE), which was originally developed at the Southern Research Institute and then subsequently enhanced by CAE. The model calculates the voltage-current characteristics and electric potential, electric field, and space charge density distributions on a two dimensional grid. These fields are in turn used to predict the particulate removal efficiency. The resistivity of the particulates is a key input in determining charge accumulation.

Stack Module. For completeness, the LEBS workbench includes a stack. At present, the stack module does not contain any models. However, models could be included to predict items such as aerosol formation, stack opacity or particulate dispersion in the local environment.

Demonstration – Prototype Workbench

To demonstrate the functionality of the prototype workbench for the LEBS-POC facility, simulations have been performed to study the impact of changes to the boiler firing conditions on the performance of other equipment located downstream of the boiler.

Steady-State Demonstration: For the test, the Overfire air and Reburn ports in the up-flow portion of the furnace have been "turned off" and the impact on the downstream equipment studied. Note that the air and fuel flows through the burners were correspondingly increased to maintain the same overall firing rate and stoichiometry. Table 1 illustrates the type of information that can be obtained. From the table it can be seen that the changed firing conditions result in reduced LOI, increased furnace exit gas temperature and a slight increase in the steam flow rate and steam temperature. For both firing conditions, the flue gas temperature at the economizer exit is about the same. The simulations also predict that the modified firing conditions increase the NOx levels at the furnace exit. In both simulations, the SCR model was run in an "iterative" manner so that the ammonia flow rate was automatically adjusted to the desired NOx level at the SCR exit (it is assumed that the NOx and ammonia levels in the flue gas exiting the SCR do not change between the SCR and the stack). For these tests, the target NOx level at the stack is the anticipated NOx regulation limit of 0.15lb/mmBTU.

From Table 1, it can be seen that the SCR operation can be modified to ensure that both firing configurations achieve the desired NOx level at the stack. However, the modified firing condition requires more ammonia to be used in the SCR. Assuming an ammonia cost of $200/ton, the increased ammonia usage results in ammonia costs increasing from $30,000/year to $54,000/year.

Table 1. Comparison of Predicted Values for Baseline Firing Conditions and Turning Off the OFA and Coal Reburn

	Baseline	**OFA & Reburn OFF**
Furnace Exit NOx, ppm dry (lb/MMBTU)	200 (0.25)	257 (0.33)
Stack NOx, ppm dry (lb/MMBTU)	119 (0.15)	119 (0.15)
Ammonia Slip, ppm dry	< 1	< 1
Ammonia Cost, $/yr	$30,000	$54,000
Steam Flow Rate, kg/s	60	66
Steam Temperature, K	1019	1025
Heat Transfer to Water Walls, MW	68	76
LOI, %	2.6	1.6
Furnace Exit CO, ppm dry	11460	7492
Furnace Exit Temperature, K	1482	1572
Economizer Gas Outlet Temperature, K	674	679
Air Heater Outlet Air Temperature, K	598	606

LEBS-POC Transient Demonstration: To demonstrate the transient capability of the *AIOLOS* reacting CFD model, a simulation for a 50% load turndown of the POC furnace has been performed. For this simulation, it is assumed that the unit is operating at 100% load and then at time t = 0, the burner fuel and air flow rates are instantaneously turned down to 50% load. The integration of the solution through time was performed in a time accurate mode. This simulation was performed by project team members at RECOM Services in Stuttgart, Germany. The computer run time required for this simulation was quite large - 76 real time hours on a single "8-processor node" of a Hitachi SR8000. The Hitachi is a hybrid supercomputer that distributes computations and memory across nodes. Within each node, the computations are performed in a SMP parallel mode across eight processors. Another high performance computer is available for these computations - the NEC SX-5 vector machine. The single node of a Hitachi is comparable to a single processor of a NEC SX-5. Using 4 NEC SX-5 processors in parallel would reduce the real time to perform this simulation by a factor of 4. It would not be practical to perform this type of simulation on a standard desktop workstation due to the long run-time required. Although *AIOLOS* is fully integrated into the workbench, to perform this simulation AIOLOS was run in "standalone" mode on the supercomputer. One of the goals of this project is to implement into the workbench environment the ability to perform CPU intensive computations on remote computers connected via a network. REI has demonstrated this capability for a relatively small model (i.e., the SCR model) using CORBA-based components. In future work we will investigate enhancing this capability to allow running large, CPU intensive simulations on a remote supercomputer or PC cluster. Here, the issues are not so much technical, but rather deal with firewalls and other security measures used at supercomputer centers.

Vision 21 Energyplex Workbench
The second workbench will contain models for simulating a Vision 21 energyplex system. As noted in the Vision 21 Roadmap, at present there is not a preferred configuration. Thus, we intend to develop models for key components that will be common to different configurations. Where possible, we will try to acquire models being developed by other Vision 21 programs. The models we intend to include in the workbench are highlighted below:

<u>Entrained Flow Gasifier</u>: This is one of the most important systems in an IGCC cycle because the gasifier converts a solid fossil fuel into more environmentally attractive hydrocarbon fuel or feedstock. Based on the reported trends in industry, we have chosen to focus on oxygen blown, entrained flow gasifiers in this project [Holt, 2001], [IEA, 2000]. Hence, with some extensions and modifications, we feel that our existing (dilute phase) CFD combustion tools can be used to model entrained flow gasifiers. Our models have been proven highly useful for evaluating large-scale industrial furnaces operating over a wide range of temperatures, stoichiometries, fuel types, and particle loadings. Many of our simulations have successfully described sub-stoichiometric environments of relevance to gasification. However, modeling the controlling phenomena in a system designed for entrained flow gasification will require the development of additional information and extensions to existing physical sub-models. We anticipate having to incorporate extensions to our models to account for high-pressure effects on the reaction kinetics and possibly the impact of the heavier particle loading. Additional models might be required to also include predictions for ash, slagging and air toxics.

Most of the validation of coal conversion phenomena depends upon experience gained at atmospheric pressure. To develop an effective gasifier model will require establishing appropriate parameters for the chemistry and physics of coal conversion phenomena at pressure and under gasification conditions. Here, we intend to collaborate with Prof. Terry Wall and other members of the Collaborative Research Center for Sustainable Development (CCSD) (formerly the Black Coal Co-operative Research Center) at the University of Newcastle, Australia. The CCSD group has extensive experience in gasification and has developed experimental data sets for pilot scale gasifier operation, reaction kinetics for high pressures and many sub-models to describe slag and ash behavior in a gasifier.

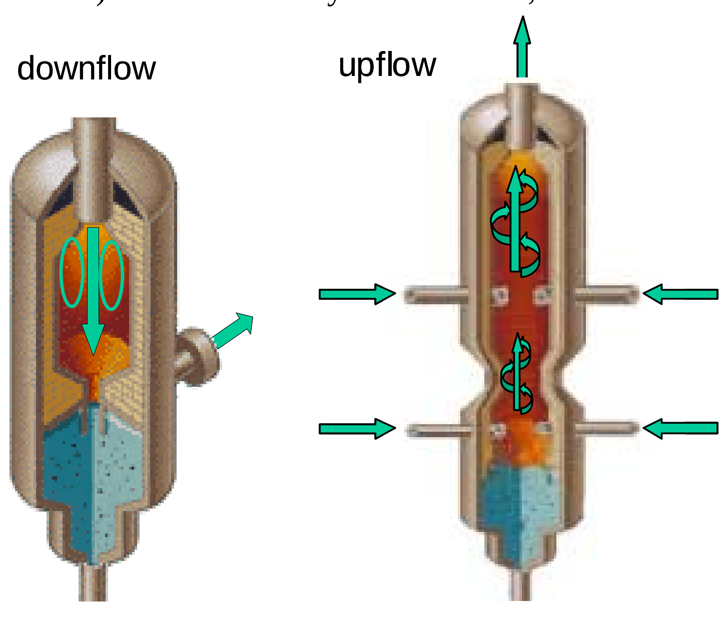

Figure 3. Generic gasifier configurations to be modeled.

It is our intention to provide within the workbench the ability to model "generic", cylindrical gasifier configurations (see Figure 3) for (1) single feed, down fired systems and (2) two stage systems with multiple feed inlets that could be opposed or tangentially fired. These systems are representative of the dominant, commercially available gasifier systems. The user will have the ability to: select different sub-models; perform limited modifications of the firing configuration, gross characteristics of the fuel injector and overall riser geometry; alter model inputs for feedstock (fuel), slurry composition and system pressure. Model outputs will include detailed information about the flowfield (e.g., gas and particle velocity, composition, temperature) and gross information about carbon conversion. The gasifier model to be developed here will allow workbench users to address many of the performance and operational problems currently hindering the operation of solid fuel gasifiers [Steigel et al, 2001], [Holt, 2001].

Fluidized Bed: We intend to include in the workbench models to simulate circulating fluidized beds. Both a reactor model and a CFD based model will be included. Implementing two models will provide users the option to use the model that best represents their system. The reactor model has the advantage of being physically realistic and runs fast enough to be used for plant design studies and possibly dynamic model response. Our reactor model will be based on previous work by [Hannes, 1993], [Glicksman et al, 1991] and [Goel, Sarofim et al, 1996]. For the CFD model we intend to use MFIX, a publicly available code developed at DOE FETC [MFIX], [Boyle, 1998], [O'Brien, 1997].

Fuel Cell **:** Fuel Cells could potentially play an important role in Vision 21 energy plants. Hence, we will include within our workbench a heat/mass balance reactor model for a Solid Oxide Fuel Cell (SOFC) for simple geometric configurations that exhibit the important fluid dynamics, heat transfer, chemical and electrochemical reactions, species transport, etc. This model will provide a simple test platform to understand the gross effects for SOFC cells. More accurate models could be developed, but would require resources beyond that available in this project.

Additional Clean Up Components: Zero dimensional reactor models will be included for an assortment of clean-up equipment, such as: candle filters, H_2S removal, particulate removal, SCR and Heat Recovery Steam Generator. The list of models to be included will be dependent on the energyplex configuration of greatest interest to the DOE. The models will be based on information and correlations available in the open literature.

Demonstration – Vision 21 Energyplex Workbench

We are working with DOE to identify energyplex configurations that are of greatest interest. As with the prototype workbench, the demonstration will be to predict system performance with the coupled modules. Key points to the tests will be to (1) exercise the user interface to determine the degree of ease-of-use, (2) exercise the improved analysis capabilities and (3) determine the impact of coupling the additional equipment into the simulation.

CONCLUSIONS

In this paper we have outlined our approach and progress for developing a computational workbench for performing virtual simulations of power plant systems. Descriptions have been provided on the functionality of the workbench and the software platform, tools and models used in the workbench. An important element in our design is the combined use of fast running reactor (process) models for some components and detailed CFD models for key components that require a detailed model. A prototype workbench based on the LEBS-POC facility has been developed and tested and efforts are now focused on developing a workbench for IGCC based energyplex systems.

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